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6. AUTHOR(S)
John E. Dennis, Jr.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Computational & Applied Mathematics
Rice University
6100 South Main Street
Houston, Texas 77005-1892

8. PERFORMING ORGANIZATION REPORT NUMBER

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13. ABSTRACT *(Maximum 200 words)*

Our paper on Mixed Variabel Pattern Search will appear in SIAM Journal on Optimization. We are awaiting referee reports on our Filter Pattern Search paper and our Analysis of Generalized Pattern Searches paper. We have received reports conditionally accepting our paper with Michael Kokkolaras, a mechanical engineering research engineer at the University of Michigan on heatshield design. In mid October, Doug Moore finished the newest release of our C++ code FOCUS. This release implements our filter pattern search method for general nonlinear programming without derivatives.

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PI: John E. Dennis, Jr.
Computational & Applied Mathematics
Rice University
6100 South Main Street
Houston, Texas 77005-1892
dennis@caam.rice.edu

CoPI: Douglas Moore
Computational & Applied Mathematics
Rice University
6100 South Main Street
Houston, Texas 77005-1892
dougm@caam.rice.edu

November 2000

Status of Effort:

Our paper on Mixed Variable Pattern Search will appear in *SIAM Journal on Optimization.* We are awaiting referee reports on our Filter Pattern Search paper and our Analysis of Generalized Pattern Searches paper. We have received reports conditionally accepting our paper with Michael Kokkolaras, a mechanical engineering research engineer at the University of Michigan on heatshield design. In mid-October, Doug Moore finished the newest release of our C++ code FOCUS. This release implements our filter pattern search method for general nonlinear programming without derivatives.

We have active collaborations with the Distributed Computing Group at Sandia Livermore Labs, Boeing Phantom Works, ExxonMobil Upstream Research, and Charles Audet of the École Polytechnique de Montréal. In addition to the new collaboration with CSRI, we will be visited in early December by representatives of the United Technology Research Center led by Mike Dorobantu to explore a collaboration on robust design and reduced subspace methods. We do our best to leverage your support.

Boeing has used our approach to design wing planforms for a new large airplane and a new small airplane.

Major Mark Abramson, USAF, has completed his comprehensive exams. He is preparing to defend his thesis proposal this winter. He will propose to extend our mixed continuous/categorical variable algorithm to handle general nonlinear constraints, implement those extensions in FOCUS, and use the code to solve a manufacturing process design problem from AFRL. Garth Frazier assures me that we will be able to get the problem even after he leaves AFRL.

We have been invited to collaborate with Bill Hart and Tony Guinta of the CSRI at Sandia Labs on an interesting mixed continuous/categorical variable problem to design the best pattern and charges for placing explosives to breach a concrete wall. This looks now to be an excellent example problem since it can be meaningfully extended to multiple objectives, robust optimization, and to a mixture of continuous, discrete, and categorical variables.

Thus, the status of the project is that it is flourishing. One upset to the status quo is that Doug Moore will leave at the end of this project to join a local dotcom. We plan to replace Doug for the proposal period with a software engineer. We are more than ever convinced that students should not be depended on for top quality software, but since Doug never participated

in the algorithmic research, we expect that his replacement should not be too difficult. Charles Audet has agreed to supervise this person, and he has identified an experienced software engineer who wishes to work in a university environment. If Doug had left last year, it would have been a serious blow, but now it is not so serious because the design of the framework has now stabilized (at least until we add categorical variables!). Our collaborators at Boeing have successfully interfaced two completely different ad hoc search routines to FOCUS, and they are happy with the results. Of course, we will stay within our budget in replacing Doug. Indeed, if we can replace him with someone at a lower salary, this will enable me to be supported at a more reasonable level.

Accomplishments/New Findings:

As we said above, the project is flourishing. We go into the renewal very pleased with what has been accomplished so far, and with some low hanging fruit to pick because of our progress this year.

- We have made a theoretical breakthrough in the analysis of generalized pattern search methods (GPS). In a 10-page paper submitted to *SIAM Journal on Optimization*, we obtain a proof of convergence of GPS for problems with general linear constraints without assuming even finite values for the objective. We identify sequences whose limit points satisfy appropriate optimality conditions depending on the local smoothness of the objective at the point.

  Thus, our result is much stronger mathematically and more practical because the functions we deal with in practice are not continuous or finite valued. Not only are our results stronger, but our proofs are much shorter. We use the Clarke generalized directional derivatives as a tool to reduce to a few lines results that took pages when published originally in *SIAM Journal on Optimization.*

- We developed a novel class of pattern search algorithms for general constrained optimization. It does not compute nor approximate any derivatives, and it does not use any penalty nor Lagrangian function. There are no penalty constants because there is no merit function. Our interest in these methods was really intensified by the fact that no

merit function means no explicit dependence on Lagrange multiplier estimates, which are a big problem for derivative-free methods.

In the original pattern search algorithms, a trial point is accepted if it reduces the incumbent objective value. Our constrained algorithm is based on the so-called filter methods of Fletcher, Leffler, and Toint. This is a new and very hot approach to globalizing SQP and SLP algorithms. A filter method accepts a trial point if it is unfiltered, i.e., if its objective function value and its constraint violation function value are not dominated in the multiobjective sense. Thus, for the unconstrained case, this reduces exactly to the previous test. Again, we are able to use Clarke's nonsmooth tools to achieve convergence without assuming continuity or finite values. We show that our algorithm generates an accumulation point satisfying first-order optimality conditions appropriate to the local smoothness of the objective and constraints at the limit point.

- Using the above filter pattern search approach, Paul Frank obtained very strong new designs of the wing planform for a new large airplane and a small airplane. The mission range constraint in the planform problem is nasty and nonlinear, so this was an excellent example to exercise our ideas. My understanding is that this will be the Boeing approach to planform design in the future. Now that is a TRANSITION.

- In mid-October, Doug Moore finished the newest release of our C++ code FOCUS. This release implements our filter pattern search method for general nonlinear programming without derivatives. It is based on a FOCUS redesign accomplished last summer during John Dennis' visit to Boeing. Boeing has successfully married the new FOCUS with two local, and quite dissimilar, Boeing favorite search routines, and they seem quite happy with the functionality of the software. The software is freely available for downloading at:
<http://www.caam.rice.edu/dougm/~focus.html>.

- Many engineering optimization problems involve a special kind of discrete variable that *can* be represented by a number, but this representation has no significance. Such variables arise when a decision involves some situation like a choice from an unordered list of categories. This has two implications: The standard approach of solving problems with

continuous relaxations of discrete variables is not available, and the notion of local optimality must be defined through a user-specified set of neighboring points.

We have a paper appearing in SIAM Journal on Optimization that defines a new class of direct search algorithms to provide limit points that satisfy some appropriate necessary conditions for local optimality for such problems. We give a more expensive, version of the algorithm that guarantees additional necessary optimality conditions. A small example illustrates the differences between the two versions.

- A real thermal insulation system design problem illustrates the efficacy of the user controls for this class of algorithms. The joint paper with Kokkolaras mentioned above as provisionally accepted in the new *Journal for Optimization in Engineering* applies our discrete/continuous direct search method MVP to obtain a greatly improved heatshield design. There are many engineering problems of this type, which until our MVP work had to be treated through parametric studies. We obtained a 65% reduction in energy use over the best published results obtained by parametric studies.

Personnel Supported:

Faculty: John Dennis
Postdoctoral Researchers: Douglas Moore
Charles Audet

Publications:

Published:

- (Natalia Alexandrov, J. E. Dennis, Jr., Robert Michael Lewis, and Virginia Torczon) "A Trust Region Framework for Managing the Use of Approximation Models in Optimization". *Structural Optimization*, 15(1), pp 16–23, 1998.
- (Andrew J. Booker, J. E. Dennis, Jr., Paul D. Frank, David B. Serafini, and Virginia Torczon. "Optimization Using Surrogate Objectives on a Helicopter Test Example". *Optimal Design and Control*, edited by J. Borggaard, J. Burns, E. Cliff, and S. Schreck, Birkhauser.
- (Indraneel Das and J. E. Dennis, Jr.) "Normal-Boundary Intersection: A New Method for Generating the Pareto Surface in Nonlinear Multicriteria Optimization Problems". *SIAM J. Optim.*, 8(3), pp 631–657, 1998.
- (J. E. Dennis, M. Heinkenschloss, and L. N. Vicente) "Trust-Region Interior-Point Algorithms for a Class of Nonlinear Programming Problems". *SIAM J. Control and Optimization*, 36(6), pp 1750–1794, 1998.
- (Charles Audet, Pierre Hansen, Brigitte Jaumard and Gilles Savard) "A Symmetrical Linear Maxmin Approach to Disjoint Bilinear Programming". *Mathematical Programming*, 85(3), pp 573–592, 1999.
- (Andrew J. Booker, J. E. Dennis, Jr., Paul D. Frank, David B. Serafini, Virginia Torczon, and Michael W. Trosset) "A Rigorous Framework for Optimization of Expensive Functions by Surrogates". *Structural Optimization*, 17(1), pp 1–13, 1999.

- (J. E. Dennis, Mahmoud El-Alem and Karen Williamson) "A Trust-Region Approach to Nonlinear Systems of Equalities and Inequalities". *SIAM J. Optim.*, 9(2), pp 291–315, 1999.

Accepted for Publication:

- (Charles Audet and J. E. Dennis) "Pattern Search Algorithms for Mixed Variable Programming", available as Rice CAAM-TR99-02, accepted for publication in *SIAM Journal on Optimization.*
- (Michael Kokkolaras, Charles Audet, and J.E. Dennis Jr.) "Mixed Variable Optimization of the Number and Composition of Heat Intercepts in a Thermal Insulation System", available as Rice CAAM-TR00-21, conditionally accepted for publication in *Journal for Optimization in Engineering.*

Submitted for Publication:

- (Natalia Alexandrov and J. E. Dennis) "A Class of General Trust-Region Multilevel Algorithms for Systems of Nonlinear Equations and Equality Constrained Optimization: Global Convergence Theory".
- (J. E. Dennis and Robert Michael Lewis) "A Comparison of Nonlinear Programming Approaches to an Elliptic Inverse Problem and a New Domain Decomposition Approach".
- (C. Audet and J. E. Dennis, Jr.) "On the Convergence of Mixed Integer Pattern Search Algorithms".
- (C. Audet) "Convergence Results for Pattern Search Algorithms are Tight", available as Rice CAAM-TR98-24.
- (Charles Audet and J. E. Dennis) "Analysis of Generalized Pattern Searches", available as Rice CAAM-TR00-07.
- (Charles Audet and J. E. Dennis) "A Pattern Search Filter Method for Nonlinear Programming without Derivatives", available as Rice CAAM-TR00-09.

Interactions and Transitions:

Public Presentations:

J. E. Dennis

- "Surrogate Optimization of Expensive Functions". Department of Mathematics & Statistics, University of Canterbury; March 19, 1998; Christchurch, NZ.
- "Trust Region Interior Point Algorithms for Engineering Design". Department of Mathematics & Statistics, University of Canterbury; March 19, 1998; Christchurch, NZ.
- "Optimization, An Essential Tool for Decision Support". Dean's Distinguished Lecture, University of Canterbury; April 7, 1998; Christchurch, NZ.
- "Surrogate Optimization of Expensive Functions". Statoil Site Visit, CITI, Rice University; April 29, 1998; Houston.
- "Rice Contributions to Research in Optimization, Automatic Differentiation, and Interior Point Methods". Distinguished Faculty Lecture, 30th Anniversary of the Rice Computational and Applied Mathematics Department; May 16, 1998; Houston.
- "Further Experiments with a Helicopter Rotor Design Problem". AIAA MDO Conference; St. Louis; September 3, 1998.
- "An Overview of Research in Optimization and Automatic Differentiation". Mobil Technology Company Site Visit; September 15, 1998.
- "Surrogate Optimization of Expensive Functions". Sandia National Laboratory; Livermore; October 1, 1998.
- "A Ferris-Mangasarian Technique Applied to Least-Squares Problems". David Young 70th Birthday Meeting; Austin; October 20, 1998.
- "Surrogate Optimization of Expensive Functions". INFORMS National Meeting; Seattle; October 26, 1998.

- "Surrogate Optimization of Expensive Functions". Department of Mathematics, Arizona State University; Tempe; February 4, 1999.
- "Surrogate Optimization of Expensive Function". Department of Energy Geophysics Workshop; San Jose; February 6, 1999.
- "Surrogate Optimization of Expensive Functions". Keynote address at German SIOPT Meeting; Trier; March 22, 1999.
- "Surrogate Optimization of Expensive Functions". Department of Mathematics, Technical University of Mexico; Mexico City; April 8, 1999.
- "Career Opportunities in Applied Mathematics". Department of Mathematics, Technical University of Mexico; Mexico City; April 9, 1999.
- "Quasi-Newton Methods from Davidon to Automatic Differentiation". Plenary talk at SIAM Optimization Meeting; Atlanta; May 10, 1999.
- "Computational and Applied Mathematics Research at Rice". Los Alamos/Rice Computer Science Institute; Santa Fe; June 7, 1999.
- "Surrogate Optimization of Expensive Functions". AFOSR Workshop on Materials Processing and Optimization; Air Force Institute of Technology, WPAFB, Dayton; July 7, 1999.
- "Optimization of Expensive Functions by Surrogates". INFORMS meeting; Cancun, Mexico; January 6, 2000.
- "Pattern Search Methods for NLP without Derivatives". University of Washington; Seattle, WA; March 6, 2000.
- "Optimization of Expensive Functions by Surrogates". ExxonMobil Upstream Research; March 31, 2000.
- "Optimization of Expensive Functions by Surrogates". INFORMS meeting; Sal,t Lake City, UT; May 7, 2000.
- "Optimization of Expensive Functions by Surrogates". CERFACS; Toulouse, France; May 25, 2000.
- "A Filter Pattern Search Method for Nonlinear Programming". CERFACS; Toulouse, France; June 1, 2000.

- "Mixed Variable Programming". CERFACS; Toulouse, France; June 8, 2000.
- "An Approach to Optimization of Pressure Driven Membrane Processes". Annual Conference of the American Water Works Association; Denver, CO; June 12, 2000.
- "A Pattern Search Filter Method for Nonlinear Programming". International Symposium on Mathematical Programming; Atlanta, GA; August 9, 2000.
- "Mixed Variable Programming". Sandia National Labs; Livermore, CA; September 13, 2000.
- "A Filter Pattern Search Method for Nonlinear Programming". Sandia National Labs; Livermore, CA; September 14, 2000.
- "Optimization-based Design Methods". AFRL/Lockheed-Martin; Orlando, FL; September 21, 2000.
- "A Rigorous Pattern Search Framework for Industrial Strength Optimization without Derivatives". First international workshop on surrogate modelling and space mapping for engineering optimization; Lingby, Denmark; November 16, 2000.
- "Generalized Pattern Search Algorithms for Mixed Variable Programming". First international workshop on surrogate modelling and space mapping for engineering optimization; Lingby, Denmark; November 17, 2000.

Douglas Moore

- "The Design of FOCUS — Framework for Optimization with Constraints Using Surrogates". Boeing; July 29, 1998; Seattle.
- "Software for Robust Optimization". Mobil Technology Company Site Visit; September 1998.
- "An Object-Oriented Framework for Surrogate-Based Optimization". AFOSR Workshop on Materials Processing and Optimization; Air Force Institute of Technology, WPAFB, Dayton; July 1999.

Charles Audet

- "Convergence of Mixed Integer Pattern Search Algorithms". GERAD Seminar; Montréal; December 1998.
- "Optimization Using Surrogates". AFOSR Workshop on Materials Processing and Optimization; Air Force Institute of Technology, WPAFB, Dayton; July 1999.
- "Analysis of Pattern Search Algorithms". CAAM Colloquium; Rice University; February 2000.
- "Derivative-free optimization for general constrained nonlinear problems". Journées de l'Optimisation 2000; Montréal, Québec; May 2000.
- "Pattern Search Algorithms for Mixed Variable Programming". CERFACS; Toulouse, France; June 2000.
- "Pattern Search Algorithms for Mixed Variable Programming". Exxon-Mobil; Houston; June 2000.
- "Analysis of Generalized Pattern Search Methods". International Symposium on Mathematical Programming; Atlanta, GA; August 9, 2000.
- "A Pattern Search Filter Method for Nonlinear Programming without Derivatives". First international workshop on surrogate modelling and space mapping for engineering optimization; Lingby, Denmark; November 16, 2000.

Consultative and Advisory Functions:

J. E. Dennis

- Spent July, 1998 at Boeing Applied Research and Technology Shared Services.
- External Advisor for University of Puerto Rico Interdisciplinary Doctoral Program in Mathematics.
- External Advisor for The University of Florida Applied Mathematics Center.
- Advisory Committee for Worcester Polytechnic Institute.

Douglas Moore

- Consulted with Juan Meza of Sandia National Laboratories (CA) on issues of numerical software design.
- Consulted with SANDIA's CSRI on engineering optimization problems.

Transitions:

Projects in the Exploratory Stage

- **Oilfield Management**

  In the last year, we continued to meet with representatives of the new ExxonMobil Upstream Co., and we helped them formulate a problem of interest to them and well-suited to the optimization techniques we are developing. This particular problem concerns the placement and management of wells in an oilfield over a 20-year period. The problem has both continuous parameters, like the placement of wells and the rates of production, and discrete ones, like the startup and shutdown dates for a given well. The problem has constraints involving bounds on production rates and interwell distances, and it incorporates both geophysical models and capital costs. We expect to continue to develop the problem and the tools to solve it over the next year. There are no continuous relaxations of the discrete parameters, and the constraints are general and involve both sorts of variables. This and the planform problem will be good test cases for algorithms that minimize a

- **Nozzle Design**

  Our group is working with a group in Boeing Commercial Airplane Group (BCAG) to reduce the cycle time for designing nozzles. A nozzle is the inside part of the engine housing, and its design is affected by the design of the more "upstream" components. This means that many of the design changes involving other airplane components force a redesign of the nozzle as well.

  A nozzle design is specified by 100 parameters, 90 of which are fixed by other considerations. The system is governed by a 2D Navier Stokes coupled with NASTRAN, a commercial structures code. It takes about 3 hours on an SGI Challenge to get one function value. The current

3 hours on an SGI Challenge to get one function value. The current length of a design cycle is two weeks. We expect to reduce that to approximately one day.

Contact: Greg Shubin (425) 865-3516.

- **High-Speed Cutting Tool Design**

  High-speed machine tools encounter the metal at over 300 mph. At that speed, the metals are not fully solid. This allows more complicated parts to be machined in a single piece. Many large airplane parts are currently assembled from components that were machined separately. If, during airplane assembly, one of these parts doesn't quite fit, work stops and a supervisor is called in to approve the use of shims to make it fit. The Boeing plant in Wichita found a significant reduction in the need for this "shimming" when large parts were machined as a single piece using a high-speed machine tool.

  Since this is a new technique, no one yet knows how to design a really good cutting tool. This is a three-variable, very expensive multiobjective problem.

  Contact: Greg Shubin (425) 865-3516.

Ongoing Projects

- **Model Management Framework Software**

  Boeing and Sandia were supplied with the C++ reimplementation, FOCUS, last spring. This implementation replaces the C++ box constrained prototype delivered previously. The framework can be used to develop model management algorithms specialized for a user's applications and capabilities.

  Contact: Greg Shubin (425) 865-3516.

- **Planform Design**

  Our group worked with another BCAG group that does planform design. We achieved better planforms with greatly reduced cycle time. The planform is the shape of the wing as viewed from above. It is a tricky design problem that involves a couple of dozen variables and some interesting constraints. For example, the fuel is outboard on the

wings, and the wings must be swept back for performance. One constraint is that the plane must not fall over backwards when the tanks are filled while the plane is on the ground. This problem involves multiple objectives and discrete variables, but the first test problem run by Boeing used cost/passenger mile as objective and assumed values for the discrete variables, like where the wings are placed on the body.

The following text on the recent test was approved by Boeing for release:

Recent Product Development activities at Boeing have underscored the need to decrease the time to market and cost of products. To accomplish this, Boeing has been examining all of its processes in development and production.

One process in particular that occurs early in the design is the determination of a wing planform, which must be chosen to meet mission while decreasing operating economics and respecting design constraints. Boeing is exploring whether this highly multi-disciplinary problem yields itself to integrated analysis and optimization techniques, with the hope of decreasing the cycle time of finding a preferred result by an order of magnitude.

This exploration provided the Design Explorer Team, of which Rice is a member, with an opportunity to apply our design optimization tools. It has also been useful from the standpoint of exercising the various discipline analysis tools. Starting from baselines developed through the standard process and using a significant subset of the tools, we have been able to demonstrate actual integration of the analyses from the different disciplines and the speed advantages that we were looking for. The solutions found do, within the level of accuracy of the included tools, meet all constraints while showing economic benefit relative to our analyses of the initial baselines.

The approach to this problem used response surface (surrogate) modeling to speed up the optimization, as opposed to continuously resampling the analysis tools. Of additional note is that incorporation of Model Management Framework elements into the optimization scheme allowed resolution of the selected optimum to search variables of second order importance. Such resolution is particularly difficult to obtain when using response surface modeling.

Contact: Greg Shubin (425) 865-3516.

- **Helicopter Rotor Blade Design**

  This is the problem we have been working on for the longest time. Wake simulation is the hard part of the problem, and the effects at the tip of the rotor blade are the most difficult to simulate. It takes about 4 hours on 16 fat nodes of an SP2. Our group at Boeing managed to build a response surface model for the spline coefficients of the output of the full potential rotor discipline as a function of the spline coefficients of the input to that code, which is the output from the coupled simulation involving thermal analysis, structural analysis, and aerodynamics analysis. This new model reduces the cost to minutes and the bandwidth of the coupling from 100s to 10s. About a year ago, we provided Boeing with the design variables corresponding to a new "best" design.

  Contact: Greg Shubin (425) 865-3516.

- **Boeing Parts Nesting System**

  PDS continues to be used in the Boeing Parts Nesting System for Just-in-Time manufacturing of aircraft parts.

Inventions, or Patent Disclosures:

None.

Honors/Awards:

J. E. Dennis

- Dedicatee of special issue of the *SIAM Journal on Optimization* (Volume 9, Number 4) <http://epubs.siam.org/sam-bin/dbq/toc/SIOPT/9/4>.
- Founder and Editor-in-Chief of MPS/SIAM Book Series on Optimization
- Advisory Editor, *Mathematics of Operations Research*, (1992—).
- Vice President of the Mathematical Programming Society.